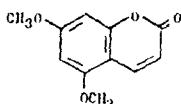


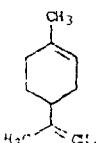
THERAP CAT: Topical antiseptic; scabicide.
THERAP CAT (VET): Insecticide, scabicide, has been used in boils and fistulas.

5332. Limettin. *5,7-Dimethoxy-2H-1-benzopyran-2-one; 5,7-dimethoxycoumarin; citropten.* $C_{11}H_{10}O_4$; mol wt 206.19. C 64.07%, H 4.89%, O 31.04%. From rind of fruit of *Citrus lima* Lunan (*C. limetta* Auth.), Rutaceae (lime); Tilden, Beck, *J. Chem. Soc.* 57, 323 (1890); from W. Indian lime oil; Caldwell, Jones, *ibid.* 1945, 570; from citrus oils; Stanley, Vannier, U.S. pat. 2,889,337 (1959 to U.S.D.A.). Synthesis: Schmidt, *Arch. Pharm.* 242, 288 (1904); Heyes, Robertson, *J. Chem. Soc.* 1936, 1831.



Needles from methanol, mp 147-148°. uv max (alcohol): 222, 247, 250.5, 324 nm (log ε 4.03, 3.84, 3.84, 4.18). Almost insol in boiling water, ether, petr ether; freely sol in alcohol, chloroform, acetone.

5333. Limonene. *1-Methyl-4-(1-methylethenyl)cyclohexene; p-mentha-1,8-diene; cineole; cajeputene; kautschin. $C_{10}H_{16}$* ; mol wt 136.23. C 88.16%, H 11.84%. Occurs in various ethereal oils, particularly in oils of lemon, orange, caraway, dill and bergamot. Isoin of d-limonene from mandarin peel oil (*Citrus reticulata* Blanco, Rutaceae); Kugler, Kováts, *Helv. Chim. Acta* 46, 1480 (1963). Review: J. L. Simonsen, *The Terpenes* vol. I (University Press, Cambridge, 2nd ed., 1947) pp 143-165.



d-Form, *inactive limonene, dipentene*. Liquid. Pleasant lemon-like odor. bp₇₆₃ 175.5-176.5°. d₄^{20.5} 0.8402. n_D²⁰ 1.4744. Practically insol in water; miscible with alcohol. With dry HCl or HBr it forms monohalides, and with aq HCl or HBr, the dihalide.

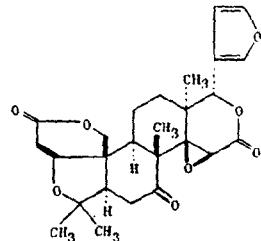
d-Form, liquid. bp₇₆₃ 175.5-176.5°. d₄²⁰ 0.8402. n_D²⁰ 1.4743. [α]_D²⁰ +123.8°.

l-Form, liquid. bp₇₆₃ 175.5-176.5°. d₄^{20.5} 0.8407. n_D²⁰ 1.474. [α]_D²⁰ -101.3°.

USE: Solvent, manuf resins; wetting and dispersing agent. Caution: Skin irritant, sensitizer.

5334. Limonin. *Limonic acid 3,19:16,17-dilactone; 8-(3-furyl)decahydro-2,2,4a,8a-tetramethyl-11H,13H-oxireno-[d]pyran[4',3':3,3a]isobenzofuro[5,4-j][2]benzopyran-4,6-,13(2H,5aH)-trione.* $C_{26}H_{30}O_6$; mol wt 470.50. C 66.37%, H 6.43%, O 27.21%. Bitter principle of lemon and other Rutaceae. Isoin: Bernays, *Ann.* 40, 317 (1841). Structure and stereochemistry: Melera et al., *Helv. Chim. Acta* 40, 1420 (1957); Arigoni et al., *Experientia* 16, 41 (1960); Arnott et al., *ibid.* 16, 49 (1960); Barton et al., *J. Chem. Soc.* 1961, 255; Arnott et al., *ibid.* 1961, 4183. Synthetic studies: Schlatter et al., *Helv. Chim. Acta* 57, 1044 (1975); Lüthy et al., *ibid.* 1060.

Limettin



Bitter crystals from methylene chloride + isopropanol or acetic acid, mp 298°. [α]_D²⁰ -128° (c = 1.21 in acetone). uv max: 207, 285 nm (ε 7000; 38). Slightly sol in water, ether; sol in alcohol, glacial acetic acid.

5335. Linalool. *3,7-Dimethyl-1,6-octadien-3-ol; 2,6-dimethyl-2,7-octadien-6-ol; linalol.* $C_{10}H_{18}O$; mol wt 154.24. C 77.87%, H 11.76%, O 10.37%. (CH₃)₂C=CHCH₂CH=C(CH₃)(OH)CH=CH₂. Chief constituent of linaloe oil; also occurs in oils of Ceylon cinnamon, sassafras, orange flower, bergamot, *Artemisia balchanorum*, ylang ylang, etc.; Tieemann, *Ber.* 31, 808 (1898); Walbaum, Stephan, *ibid.* 33, 2305 (1900); Hesse, Zeitschel, *J. Prakt. Chem.* 66, 493 (1902); Rafanova et al., U.S.S.R. pat. 103,725 (1956); C.A. 51, 3656c (1957); Naves, *Helv. Chim. Acta* 42, 1692 (1959). Presence in essential oils: *idem, Compt. Rend.* 251, 900 (1960). Absolute configuration: Prelog, Watanabe, *Ann.* 603, 1 (1957). Synthesis of *dl*-linalool: Ruzicka, Fornasir, *Helv. Chim. Acta* 2, 182 (1919); Surmatis, U.S. pat. 2,848,502 (1958 to Hoffmann-La Roche); Nair, Pandit, *Tetrahedron Letters* 1966, 5097. Review: J. L. Simonsen, *The Terpenes* vol. I (University Press, Cambridge, 2nd ed., 1947), pp 57-68.

l-Form, *licareol*. Colorless liq. bp₇₆₀ 198°; bp₂₀ 98-98.3°; bp₁₀ 86-87°. d₂₀²⁰ 0.8622. n_D²⁰ 1.4604. [α]_D²⁰ -20.1°. Practically insol in water; miscible with alcohol, ether.

d-Form, *cortandrol*. bp₇₆₀ 198-200°; bp₂₀ 114-114.5°; bp₁₀ 93-94°; bp₁₀ 86°. d₂₀²⁰ 0.8733. n_D²⁰ 1.4673. [α]_D²⁰ +19.3°. Soluble in 10 vol 50% alc, 4 vol 60% alc.

dl-Form, bp₇₆₀ 194-197°; bp₁₀ 89-91°. d₂₀²⁰ 0.865.

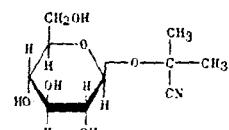
USE: In perfumery instead of bergamot or French lavender oil since it has an odor similar to these oils.

5336. Linallyl Acetate. *3,7-Dimethyl-1,6-octadien-3-yl acetate; bergamot.* $C_{11}H_{18}O_2$; mol wt 196.28. C 73.43%, H 10.27%, O 16.30%. CH₃COOC₁₀H₁₇. Most valuable constituent of bergamot and lavender oils, also found in many other volatile oils.

Liquid: bergamot odor. d₂₀²⁰ 0.895. bp 220°. n_D²⁰ 1.4460. Insol in water; miscible with alcohol, ether.

USE: In perfumery.

5337. Linamarin. *2-(β-D-Glucopyranosyloxy)-2-methylpropanenitrile; phaseolinatin.* $C_{19}H_{21}NO_6$; mol wt 247.24. C 48.58%, H 6.93%, N 5.67%, O 38.83%. From the seed skins or embryos of flax: Jorissen, Hairs, *Bull. Acad. Roy. Sci. Belg.* [3] 21, 529 (1891); André et al., *Compt. Rend.* 231, 590 (1950); Lüdtke, *Biochem. Z.* 323, 428 (1953). Synthesis: Fischer, Anger, *Ber.* 52, 854 (1919). Biosynthesis in white clover: Butler, Butler, *Nature* 187, 780 (1960).



Bitter needles, mp 142-143°. [α]_D²⁰ -29°. Freely sol in water, cold alcohol, hot acetone; slightly in hot ethyl acetate, ether, benzene, chloroform; practically insol in petr ether. Evolves HCN with linseed meal but not with emulsin.

Tetraacetate, $C_{23}H_{25}NO_{10}$, needles from alcohol, mp 140-141°. [α]_D²⁰ -10.8° (acetone). Sol in acetone, ethyl acetate, chloroform, glacial acetic acid, benzene, warm methanol and ethanol; practically insol in petr ether.

A
w
P

p/
la
H
23
lin
19:
U.S.
joh
42:
3,3
hec